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# Spitzer Spectroscopy of Ices: From Molecular Cores to Planet-Forming Disks

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**Abstract.** Icy grain mantles are a major reservoir of the molecular inventory of dense clouds and circumstellar envelopes and disks. The ice abundances and in particular the dependence of abundances on the astrophysical environment are still poorly characterized. Numerous physical and chemical processes may modify the ices in the evolutionary sequence from dense cores to planet-forming disks. Using Spitzer/IRS and ground-based thermal infrared spectrometers we determine the ice inventory toward low mass protostars and address questions on evolutionary scenarios. The initial results from our Spitzer Legacy program "From Molecular Cores to Planet-Forming Disks" (*c2d*) indicate that ice abundances relative to $H_2O$ commonly vary by factors of 2–5 in different sight-lines. For some species (CO) outgassing is likely responsible, but for others ($CH_3OH$, $CO_2$, $NH_3$) different factors, such as cloud history, must be involved.

## 1. Introduction

Infrared spectroscopic observations of the vibrational modes of ices revealed the presence of $H_2O$, CO, $CO_2$, OCS, $CH_3OH$, HCOOH, $H_2CO$, and $CH_4$ in dense clouds and the envelopes surrounding high and low mass protostars (e.g. Boogert & Ehrenfreund 2004[1]). The observations are heavily biased to objects with bright continuum emission and the sample sizes are small. It is thus still unclear if the abundances of these simple species vary between objects of similar mass and age and between classes of objects. Such knowledge is highly relevant, as laboratory studies have shown that these simple species may well be the basis for the formation of more complex species (PAHs, amino acids, hydrocarbons; Bernstein et al. 2002, Greenberg et al. 2000). A suite of processes, ranging from heating, to cosmic ray bombardment, to irradiation by ultraviolet photons, could accomplish this. The relevance of these processes in the astrophysical environment can be investigated by observing ices directly over the entire evolutionary range of star formation: from background stars tracing quiescent dense cloud material, to the envelopes of deeply embedded Class 0 and 1 protostars, to the disks surrounding Class 2 objects. With the availability of the sensitive IRS spectrometer (Houck et al. 2004) on board the Spitzer Space Telescope (Werner et al. 2004) this is now possible for the first time. Here we present the initial results of our *c2d* Spitzer Legacy program (Evans et al. 2003).

[1] see also http://www.astro.caltech.edu/∼acab/icefeatures.html

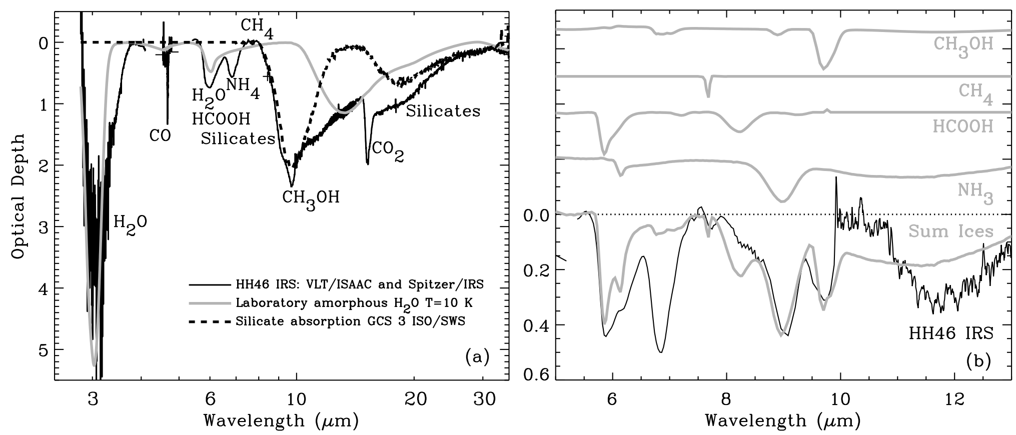


Figure 1. **(a):** Combined Spitzer/IRS and VLT/ISAAC 2-33 $\mu$m spectrum of the low mass protostars HH46 IRS on an optical depth scale. A pure solid $H_2O$ laboratory spectrum at $T$ =10 K (Hudgins et al. 1993) is fit to the data, as well as the silicate absorption spectrum of GCS 3 (Chiar et al. 2000). **(b):** Mid-infrared spectrum of HH46 IRS after subtraction of those $H_2O$ and silicate spectra. Absorption features are identified using the labeled individual and composite (bottom) laboratory spectra. No attempt was made to fit the 6.85 $\mu$m band (possibly $NH_4^+$). Also, the shape of the feature at 11.7 $\mu$m is unreliable due to large corrections for the $H_2O$ libration mode.

## 2. Ice Inventory

The O–H and C–H bending mode vibrations occur typically at the wavelengths at which Spitzer/IRS operates (>5 $\mu$m), and the stretching mode vibrations at 3-5 $\mu$m. To de-blend the multitude of absorption features it is essential that the full 3-20 $\mu$m region is studied. Therefore complementary ground-based 3-5 $\mu$m spectra are being obtained. Numerous ice absorption features are present, which we highlight by subtracting the main absorbers, i.e. $H_2O$ ice and silicates, on optical depth scale (Fig. 1a). When the laboratory $H_2O$ ice spectrum is scaled to the observed 3 $\mu$m absorption band, the 6 $\mu$m absorption feature is only partially (50%) explained by the $H_2O$ bending mode; this was also observed for high mass protostars (Schutte et al. 1996). Our subtraction of the silicate contribution is rudimentary, but serves the purpose of this presentation. The silicate bands toward the diffuse medium source GCS 3 were used as a template (Chiar et al. 2000). The excess absorption spectrum in the 5-14 $\mu$m region (i.e. without $H_2O$ and silicate contributions) is a rich blend of features (Fig. 1b). All of the detected features are real, but especially above 8 $\mu$m the profile shapes are still somewhat uncertain. The identification and abundances are determined using a set of laboratory ice spectra. Within our sample of 5 low mass protostars, and compared to previously studied high mass protostars, abundance variations of a factor of 2 are common for $CO_2$, $CH_4$, and HCOOH (Table 1). Larger variations (factor ∼5) are seen for $CH_3OH$, CO, and possibly $NH_3$. In particular the presence and abundance of $NH_3$ needs further study by combining information from the various features throughout the spectrum, as each band is strongly blended with other features (e.g. Taban et al. 2003).

Table 1. Ice abundances covering both low and high mass protostars and background stars. Species in brackets are uncertain identifications.

| Species | Abundance % of $H_2O$ | Species | Abundance % of $H_2O$ |
|---|---|---|---|
| CO | few-50 | OCS | $< 0.05$, 0.2 |
| $CO_2$ | 15-35 | ($NH_3$) | $< 10$, 40 |
| $CH_4$ | 2-4 | ($HCOO^-$) | 0.3 |
| $CH_3OH$ | $< 8$, 30 | ($SO_2$) | $\leq 3$ |
| HCOOH | 3-8 | ($NH_4^+$) | 3-12 |
| $H_2CO$ | $< 2$, 7 | ($OCN^-$) | $< 0.2$, 7 |

## 3. Ice Composition Evolution?

No particular trend in ice abundances with protostellar age is evident, except for an overall reduction in abundance due to sublimation in the least embedded (oldest) systems. The most volatile species sublimate at earlier times, as evidenced by the profile of the CO stretch mode of 4.67 $\mu$m, where the 'apolar' CO component disappears first (e.g. Boogert et al. 2002). Although the relative strength of the CO components varies, always the same components are observed (Pontoppidan et al. 2003), which shows that the formation of new species in the CO ice (e.g. $CO_2$) by energetic processes is not efficient. Indeed, the evidence for ice heating is much stronger compared to the evidence for energetic processing. For high mass protostars a comprehensive set of ice and gas temperature tracers proved that thermal processing of protostellar envelopes progresses with age: higher gas/solid state abundance ratios, more $H_2O$ ice crystallization, lower ratio of 'apolar/polar' CO components, larger warm gas phase fractions, lower ice abundances (Boogert et al. 2000, van der Tak et al. 2000). Similar effects are now observed toward low mass protostars as well, and although the sample size is still small, a tentative trend with age (traced by embeddedness) is observed. For example, an increased degree of ice crystallization is traced by the profile of the $CO_2$ bending mode. Such ice heating is also observed in edge-on disks, presumably in the heated, flared, disk surface layers that are traced at the slight inclinations required to observe the central star (Boogert et al. 2002, Pontoppidan et al. 2005). Knowledge of source geometry and orientation is crucial in the interpretation of ice observations (e.g. separation from age effects).

Not all observed abundance variations (§2) can be explained by ice heating however. The $CO_2$, $CH_3OH$, and $CH_4$ variations are possibly related to different cloud conditions at the time of the ice formation (C/CO ratios; e.g. Pontoppidan et al. 2004). Most notable is the $CO_2/H_2O$ abundance ratio, which appears to be a factor of two larger toward many low mass stars (Nummelin et al. 2001, Boogert et al. 2004) compared to the value of 17% observed toward high mass protostars (Gerakines et al. 1999). Also qualitatively the $CO_2$ ices appear to be different: the profile of the 15 $\mu$m bending mode indicates an additional apolar (pure $CO_2$ or $CO/CO_2$) component as well not seen toward massive protostars. The same $CO_2$ bending mode profile indicates that little $CH_3OH$

is mixed in the ices toward two low mass Class 1 protostars (Boogert et al. 2004). On the other hand, whereas high $CH_3OH$ abundances previously seemed exclusively associated with some high mass protostars (Dartois et al. 1999), a large $CH_3OH$ concentration is now detected in the envelope of one Class 0 source as well ($CH_3OH/H_2O/\sim25\%$; Pontoppidan et al. 2004). It is yet unclear whether this is a transient effect in the protostellar evolution or a result of specific native cloud history.

## 4. Conclusions

Full spectroscopic coverage of the 2-20 $\mu$m region with the sensitive Spitzer/IRS and ground based spectrometers allows for the first time a determination of the inventory of ices toward low mass protostars. Abundance variations by factors of 2-5 between high and low mass protostars and among low mass protostars are clearly observed. We tentatively conclude that the chemical and physical history of the native cloud is more important in the formation of simple species ($CO_2$, $NH_3$, $CH_3OH$) than is the effect of increasing exposure to energetic processes at increasing protostellar age. If true, different initial conditions in different clouds (such as the $NH_3/CH_3OH$ ratio) may profoundly affect the formation of more complex species, as different classes of molecules are formed from $NH_3$ and from $CH_3OH$ (Cazaux et al. 2003). In contrast, it appears that, as for high mass protostars, thermal processing (heating) with age is readily observed by ice crystallization and evaporation. As part of the '*c2d*' Legacy program a much larger sample ($\sim$30) of low mass protostars and background stars will be observed, allowing us to draw firmer conclusions on the origin of abundance variations and the formation processes of complex species.

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